Electron-impact excitation and dissociation processes in H_2

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The electron-impact excitation and dissociation cross sections for the $C\,^1\Pi_u$, $c\,^3\Pi_u$, $B'\,^1\Sigma_u^+$, and $E(F)\,^1\Sigma_g^+$ states of H_2 have been calculated within the distorted-wave approximation. The distorted waves are obtained as solutions of the static-exchange potential field of the ground electronic state. Both differential and integral inelastic cross sections are reported and compared with other calculated results and available experimental data.

I. INTRODUCTION

Electron-impact-induced excitation and dissociation processes in molecules play an important role in many fields of physics and chemistry, such as laser physics, astrophysics, atmospheric physics, and photochemistry. *Ab initio* theoretical methods are clearly of interest in view of the difficulties in obtaining experimental measurements of such cross sections and of the need for theoretical results in the interpretation and analysis of experimental results, e.g., in converting relative measurements to an absolute scale. Theoretical methods can also be used to obtain estimates of the contribution of higher-lying states to several processes. Such contributions can often be very difficult to measure experimentally.

In contrast to the rapid development of methods for elastic electron-molecule collision,[1,2] limited progress has been made in inelastic scattering problems involved in molecular electronic excitation and dissociation processes. Until quite recently, the Born approximation and its modified versions[3-7] were the only practical methods for studying such problems. For this reason, there is considerable interest in developing more accurate methods that can be extended to low impact energies where "plane-wave" methods are known to fail. Recently, Chung and Lin and co-workers[8,9] applied the two-state close-coupling approximation to several electronic transitions in H_2 and N_2. Hazi[10] has applied the impact-parameter method to several transitions from the ground state of H_2, F_2, and N_2. McKoy and co-workers[11-15] have applied a distorted-wave (DW) method in which the elastic scattering wave functions were obtained from an approximate solution of the Lippmann-Schwinger equation with the static-exchange potential. These results showed that the DW method can provide results which are both qualitatively and quantitatively useful when comparisons with available experimental data are made.

Recently, Lucchese *et al.*[16] have developed an iterative approach to the solution of the Lippmann-Schwinger scattering equation which is based on the Schwinger variational principal. Applications have shown that the method is an effective approach for obtaining elastic scattering wave functions at the static-exchange level. This procedure should allow the DW method to be applied more extensively than previously possible. In this paper, we will use this approach to extensively study the electronic excitation and dissociation processes in H_2 by the electron impact within the distorted-wave approximation.

There has been renewed interest in the electron-impact excitation cross sections in H_2 in part due to the detection of the intense auroral emission from Jupiter by the Voyager I and II spacecrafts. The modeling of Jovian aurora,[17-19] which offers a straightforward way of understanding the nature of the Jovian atmosphere, requires the knowledge of these cross sections. In particular, we will present cross sections for excitation of the $C\,^1\Pi_u$, $c\,^3\Pi_u$, $B'\,^1\Sigma_u^+$, and $E(F)\,^1\Sigma_g^+$ states from the ground state of H_2. We have also calculated cross sections for production of $H(2s)$ metastable atoms via dissociation of the $B'\,^1\Sigma_u^+$, $E(F)\,^1\Sigma_g^+$, and $e\,^3\Sigma_u^+$ states.

In Sec. II, we briefly discuss the theoretical formulation of our approach. In Sec. III, we discuss some aspects of the calculations and compare our results with the available experimental values and with other theoretical methods. Finally, in Sec. IV, we present our conclusions.

II. THEORY

In this section, we will present only briefly the formulation used in these studies. A detailed description of the method has been given previously by Fliflet and McKoy.[16]

In the Born-Oppenheimer and Franck-Condon approximations, and assuming the target rotational levels to be essentially degenerate, the differential cross section for electronic excitation by electron impact can be expressed in the form

$$\frac{d\sigma}{d\Omega}(n\leftarrow 0;E,\hat{r}')=SM\sum_{\nu'}\frac{k_{\nu'}}{k_0}q_{\nu'0}\frac{1}{8\pi^2}\int d\hat{R}'\,|f_{k_0}(n\leftarrow 0;\vec{R}',\hat{r}')|^2 \tag{1}$$

for incident energy $E=\frac{1}{2}k_0^2$. In Eq. (1) $f_{k_0}(n\leftarrow 0;\vec{R}',\hat{r}')$ is the fixed-nuclei scattering amplitude in the laboratory frame with the z' axis in the direction of the incident electron beam, $\vec{R}'$ denotes the nuclear coordinates of the target, and $\hat{r}'$ the scattering angles. The $q_{\nu'0}$ is the Franck-Condon factor between the $\nu=0$ vibrational level of the ground state and the ν' level of the excited electronic state, and k_0 and $k_{\nu'}$ are the momentum of the incident and scattered electrons, respectively. Equation (1) implicitly neglects the dependence of the scattering amplitude on the vibrational level of the final target state. For linear molecules M is the orbital angular momentum projection degeneracy factor of the final target state (one for a Σ state and two for a Π state). Finally, the factor S comes from summing over final and averaging over initial spin sublevels, and S is $\frac{1}{2}$ for singlet-to-singlet transition and $\frac{3}{2}$ for singlet-to-triplet excitation.

The scattering amplitude is treated within the distorted-wave approximation which is readily derived from the two-potential formula.[20] The electronic portion of the transition matrix in the body-fixed frame is given by

$$\langle k_n,n\,|\,T_{\rm el}\,|\,k_0,0\rangle=\langle\phi_n\Psi_{kn}^{(-)}\,|\,U\,|\,\phi_\alpha\Psi_{k_0}^{(+)}\rangle_a\ , \tag{2}$$

where $\Psi_{k_0}^{(+)},\psi_{kn}^{(-)}$ are initial and final Hartree-Fock (static-exchange) continuum spin orbitals, satisfying outgoing-wave and incoming-wave boundary conditions, respectively; ϕ_α is a Hartree-Fock occupied spin-orbital, ϕ is a spin-orbital of the V^{N-1} potential formed by removing an electron from the target orbital α, and U is the transition potential operator defined as

$$U=\sum_{i=1}^{N}\frac{2}{r_{i,N+1}}\ . \tag{3}$$

The antisymmetrized matrix element is defined as

$$\langle ij\,|\,U\,|\,kl\rangle_a=\langle ij\,|\,U\,|\,kl\rangle-\langle ij\,|\,U\,|\,lk\rangle\ . \tag{4}$$

The initial and final continuum space orbitals are expanded in partial-wave series:

$$\Psi_{\vec{k}_0}^{(+)}(\vec{r})=\left[\frac{2}{\pi}\right]^{1/2}\sum_{lm}i^l\psi_{k_0lm}^{(+)}(\vec{r})Y_{lm}(\hat{k}_0)\ , \tag{5a}$$

$$\Psi_{\vec{k}_n}^{(-)}(\vec{r})=\left[\frac{2}{\pi}\right]^{1/2}\sum_{lm}i^l\psi_{k_nlm}^{(-)}(\vec{r})Y_{lm}(\hat{k}_n)\ . \tag{5b}$$

This leads to a single-center expansion of the transition matrix element in the body-fixed frame of the form

$$\langle k_n,n\,|\,T_{\rm el}\,|\,k_0,0\rangle=\sum_{ll'mm'}i^{l-l'}\langle k_nlm,n\,|\,T_{\rm el}\,|\,k_0l'm',0\rangle Y_{lm}(\hat{k}_n)Y_{l'm'}(\hat{k}_0)\ . \tag{6}$$

The laboratory-frame differential cross section in the j_t basis expansion, after orientational averaging, is given by

$$\frac{d\sigma}{d\Omega}(n\leftarrow 0)=SM\sum_{\nu'}\frac{k_{\nu'}}{k_0}q_{\nu 0}\sum_{j_tm_tm_t'}\frac{1}{2j_t+1}\,|B^{j_t}_{m_tm_t'}(n\leftarrow 0,k_0,\vec{R}',\hat{r}')|^2\ , \tag{7}$$

where $\vec{j}_t$ is the angular momentum transfer for the collision, i.e.,

$$\vec{j}_t=\vec{l}-\vec{l}'\ , \tag{8}$$

and $B^{j_t}_{m_t m_{t'}}(n\leftarrow 0,k_0;\vec{R}',\hat{r}')$ is the j_t-basis expansion coefficient which can be related to the fixed-nuclei dynamical coefficients by

$$B^{j_t}_{m_t m_{t'}}(\Omega')=\sum_{ll'mm'}(-1)^{m'}a_{ll'mm'}(l'l,0m_t\,|\,j_t m_t)(l'l,-m'm\,|\,j_t m_{t'})Y_{lm_t}(\Omega')\ . \tag{9}$$

For linear molecules m_t, the projection of j_t, is determined by the states involved in the transition, and the fixed-nuclei dynamical coefficients $a_{ll'mm'}$ are given by

$$a_{ll'mm'}(n\leftarrow 0,k_0,r)=-\tfrac{1}{2}\pi\sqrt{4\pi(2l'+1)}\,i^{l'-l}\langle k_n lm,n\,|\,T_{\rm el}\,|\,k_0 l'm',0\rangle\ . \tag{10}$$

To obtain the continuum orbitals $\Psi^{(-)}_{k_n lm}$ and $\Psi^{(+)}_{k_0 l'm'}$ we use the method based on the Schwinger variational principle which has been previously discussed by Lucchese *et al.*[21] The iterative Schwinger variational method is an approach for solving the partial-wave Lippmann-Schwinger equation

$$\psi^{(+)}_{klm}=\phi_{klm}+G^{(+)}(E)U\psi^{(+)}_{klm}\ , \tag{11}$$

where ϕ_{klm} is a component of the incident plane wave, $G^{(+)}$ is the free-particle Green's function with outgoing-wave boundary conditions, $U=2V$, and V is the scattering potential. The partial-wave component of the total scattering wave function is defined by

$$\psi^{(\pm)}_{\vec{k}}=\left[\frac{2}{\pi}\right]^{1/2}\sum_{lm}i^l\psi^{(+)}_{klm}(\vec{r})Y^*_{lm}(\Omega_{\hat{k}})\ . \tag{12}$$

Expansion of the scattering wave function ψ_{klm}, in basis functions $\{\alpha_i\}$, and variation of the linear expansion coefficients lead to the Schwinger variational result

$$T_{ll'm}=\sum_{\alpha_i,\alpha_j}\langle\phi_{klm}\,|\,U\,|\,\alpha_i\rangle[(D^{(+)})^{-1}]_{ij}\langle\alpha_j\,|\,U\,|\,\phi_{kl'm}\rangle\ , \tag{13}$$

where

$$D^{(+)}_{ij}=\langle\alpha_i\,|\,U-UG^{(+)}U\,|\,\alpha_j\rangle\ . \tag{14}$$

The corresponding approximate scattering solution of Eq. (10) is then

$$\tilde{\psi}_{klm}(\vec{r})=\phi_{klm}(\vec{r})+\sum_{\alpha_i,\alpha_j}\langle\vec{r}\,|\,G^{(+)}U\,|\,\alpha_i\rangle(D^{-1})_{ij}\langle\alpha_j\,|\,U\,|\,\phi_{klm}\rangle\ . \tag{15}$$

We have developed a method to iteratively improve the scattering wave function in Eq. (16). This procedure[16] can be used to obtain the correct solutions of the scattering equations for a given potential U.

III. CALCULATION AND RESULTS

For the scattering potential, we use the static-exchange potential where the target wave function was obtained from self-consistent-field (SCF) calculation using a [5*s* 2*z*] Cartesian Gaussian basis.[22] The SCF energy for H_2 in this basis is -1.1330 a.u. and the quadrupole moment is $-0.454\,35$ a.u. at an internuclear distance of 1.4006 a.u.

The basis set used to obtain the scattering wave functions in this calculation has been given elsewhere.[16] For this simple system and this basis set no additional steps were required in the iterative procedure.

A. Excitation processes

For the final target excited states we used a frozen-core approximation for the $N-1$ unexcited orbitals and the excited orbitals was obtained as an eigenfunction of the V_{N-1} potential of this core.[23] The basis set used for the determination of these excited orbitals is shown in Table I and consists of a [7*s* 7*z*] Cartesian Gaussian basis contracted from a [10*s* 7*z*] basis. With this basis set, the calculated vertical excitation energies for the $c\,^3\Pi_u$, $C\,^1\Pi_u$, $E(F)\,^1\Sigma_g^+$, and $B'\,^1\Sigma_u^+$ states of H_2 are 12.19, 13.09, 13.32, and 14.67 eV, respectively. These can be compared with the experimental values[24] of 12.7,

TABLE I. Basis functions used in the calculation of the excited states.

S		P	
Exponent	Coefficient	Exponent	Coefficient
1685.517	0.004 227	4.8	1.0
249.958 4	0.035 026	2.53	1.0
55.658 34	0.192 039	1.33	1.0
15.274 3	0.833 376	0.733 825	1.0
4.862 8	1.0	0.174 211	1.0
1.731 6	1.0	0.055 713	1.0
0.668 05	1.0	0.020 185	1.0
0.274 37	1.0		
0.116 98	1.0		
0.041 133	1.0		

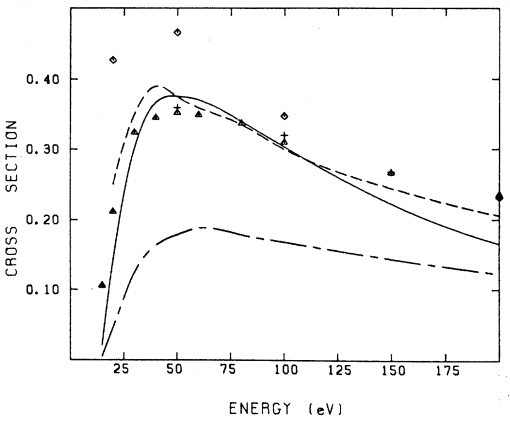

FIG. 1. Integral cross section (in 10^{-16} cm^2) for excitation of the $C\,^1\Pi_u$ state: the DW results (solid line); the Born-Ochkur results of Ref. 3 (dashed line); the Born cross sections of Ref. 7 (open diamonds); the semiempirical results of Ref. 28 (long-short dashed line); the emission experimental data of Ref. 18 (open triangles) and of Ref. 27 (crosses).

13.5, 13.1, and 14.8 eV, respectively.

To calculate the distorted-wave matrix elements

$$\langle \Psi^P_{k_n}\phi_n \mid U \mid \phi_0\psi^P_{k_0}\rangle\ , \tag{16}$$

we make use of single-center expansions for the continuum wave functions, the target orbitals, and the transition potential operator. Sufficient terms in these expansions are included to converge each partial- distorted-wave matrix element to three significant figures and the radial integrals are evaluated by Simpson's rule quadrature. In this calculation, we included partial-wave matrix elements for $l,l' \leq 6$, $m,m' \leq 1$. For singlet-singlet transitions, contributions from higher-partial-waves to the direct matrix elements are then included in the Born approximation in the way described by Fliflet and McKoy[13]; as the exchange part of the partial-wave matrix elements converge rapidly, no higher-order corrections are included for these elements. We estimate that the contribution to the differential cross section from higher-partial-wave matrix elements is less than 5% at the impact energies considered in this work. The overall numerical uncertainty in these results is about 10%.

We use the Franck-Condon factors calculated by Cartwright[25] for the transitions $X\,^1\Sigma_g^+(v=0)\rightarrow C\,^1\Pi_u$, $X\,^1\Sigma_g^+(v=0)\rightarrow c\,^3\Pi_u$, and $X\,^1\Sigma_g^+(v=0)\rightarrow E(F)\,^1\Sigma_g^+$; for the transition $X\,^1\Sigma_g^+(v=0)\rightarrow B'\,^1\Sigma_u^+$, the Franck-Condon factors of Spindler[26] have been used. Adequate convergence of the sum over v_n was obtained by including only the Franck-Condon factors for the discrete vibrational levels.

Our integral cross sections for excitation of the $C\,^1\Pi_u$, $c\,^3\Pi_u$, $E(F)\,^1\Sigma_g^+$, and $B'\,^1\Sigma_n^+$ states are shown in Figs. 1 through 4. In Fig. 1, we also show the experimental results for the $C\,^1\Pi_u \rightarrow X\,^1\Sigma_g^+$ transition obtained from uv emissions of H_2 induced by electron impact.[18,27] The agreement, in general, is good for the entire energy range of this calculation (15—200 eV). We also compare our results to those obtained by the Born,[7] Born-Ochkur,[3] and semiempirical approximations[28] In the semiempirical approximation, the cross section is expressed in an analytical form given as

$$\sigma = \frac{q_0 A}{W}\left[\frac{W}{E}\right]^{\Omega}\Phi\ , \tag{17}$$

where Φ is a phenomenological distortion factor that is incorporated to correct the Born approximation at low impact energies. This factor Φ is given by

$$\Phi = 1-\left[\frac{W}{E}\right]^{\gamma} \tag{18a}$$

for singlet-triplet transitions and

$$\Phi = \left[1-\frac{W}{E}\right]^{\nu} \tag{18b}$$

for singlet-singlet transitions. W is the excitation energy, E the incident energy, and q_0 is a constant equal to 6.514×10^{-14} cm^{2}eV^2; A, Ω, γ, and ν are adjustable parameters. In this work, the semiempirical integral cross sections are obtained from Eq. (15) using the published parameters of Ref. 28.

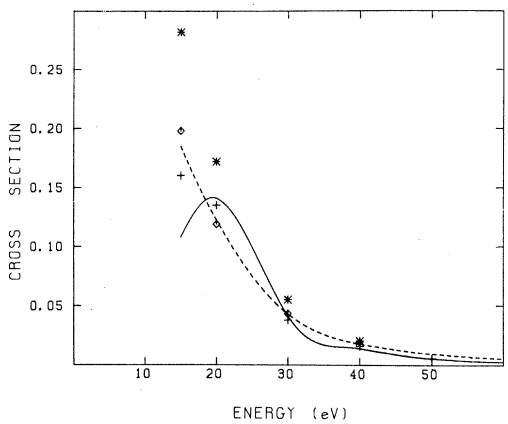

FIG. 2. Integral cross section (in 10^{-16} cm^2) for excitation of the $c\ ^3\Pi_u$ state: the present DW results (solid line); Born-Ochkur-Rudge results of Ref. 6 (open diamonds) and of Ref. 3 (crosses); the two-state close-coupling results of Ref. 8 (scaled down by a factor of 0.5, stars); and the semiempirical results of Ref. 28 (dashed line).

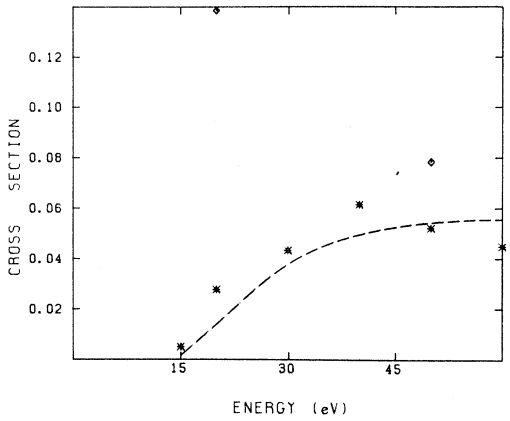

FIG. 3. Integral cross section (in 10^{-16} cm^2) for excitation of the $E(F)\ ^1\Sigma_g^+$ state: the DW results (stars), the Born cross section of Ref. 7 (open diamonds), and semiempirical data of Ref. 28 (dashed line).

One can see that the integral cross sections of the Born-Ochkur approximation agree very well with ours, and the Born results are generally higher than ours by about 20%. The semiempirical results of Miles *et al.*[28] are lower than ours by a factor of about 2 at 50 eV. This discrepancy diminishes with the increasing impact energy. For the transition $X\ ^1\Sigma_g^+ \rightarrow c\ ^3\Pi_u$, shown in Fig. 2, there are no measurements in the present energy range and hence we only compare our results with other calculated cross sections and with the semiempirical cross sections of Miles *et al.*[28] For impact energies greater than 20 eV, our results agree very well with the semiempirical estimates[28] of these cross sections and with the Born-Ochkur[3] and Born-Rudge[5] calculations. For this excitation, the two-state close-coupling (CC) approximation used by Chung and Lin[8] gives cross sections much larger than those obtained by other theoretical approaches. Although the discrepancy diminishes with increasing incident energy, the close-coupling result is still larger than the results of other approximate methods by a factor of 2 at 40 eV. We can offer no particular reason for this discrepancy.

Figures 3 and 4 show the cross sections for the $X\ ^1\Sigma_g^+ \rightarrow E(F)\ ^1\Sigma_g^+$ and $X\ ^1\Sigma_g^+ \rightarrow B'\ ^1\Sigma_u^+$ excitations, respectively. We do not know of any experimental determination of these cross sections, and theoretical estimates have only been obtained using a semiempirical method[28] and in the Born approximation.[7] Our cross sections for the $X\ ^1\Sigma_g^+ \rightarrow$ $E(F)\ ^1\Sigma_g^+$ excitation agree very well with the semiempirical estimates. The $X\ ^1\Sigma_g^+ \rightarrow B'\ ^1\Sigma_u^+$ cross sections also agree well with the semiempirical results at incident energies up to 60 eV. A comparison of the present DW results with the Born results in both cases shows that the Born cross sections are much larger than ours, but, as expected, this discrepancy diminishes with increasing incident energy.

The differential cross sections of these various transitions at incident energies of 20 and 60 eV are shown in Figs. 5 and 6. These differential cross sections have not been studied experimentally but their qualitative behavior seems quite reasonable. For more quantitative comparisons, absolute experimental measurements of these transitions would be required.

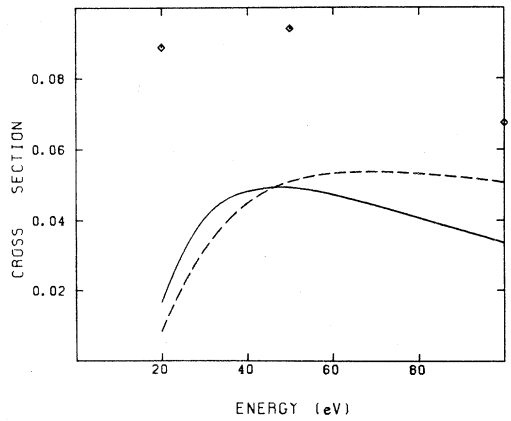

FIG 4. Integral cross sections (in 10^{-16} cm^2) for excitation of the $B'\ ^1\Sigma_u^+$ state: the DW results (solid line); Born cross sections of Ref. 7 (open diamonds) and semiempirical results of Ref. 28 (dashed line).

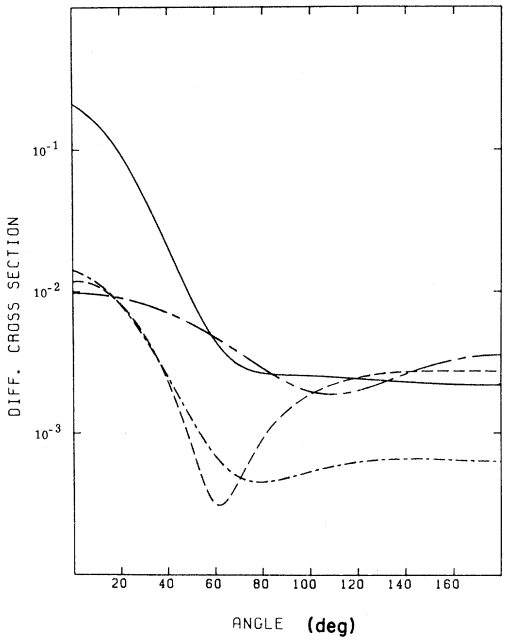

FIG. 5. Differential cross sections (in 10^{-16} cm^2/sr) for excitations of the $C\,^1\Pi_u$ (solid line); $c\,^3\Pi_u$ (long-short dashed line); $E(F)\,^1\Sigma_g^+$ (dashed line) and $B'\,^1\Sigma_u^+$ (dashed-dot line) states at 20 eV.

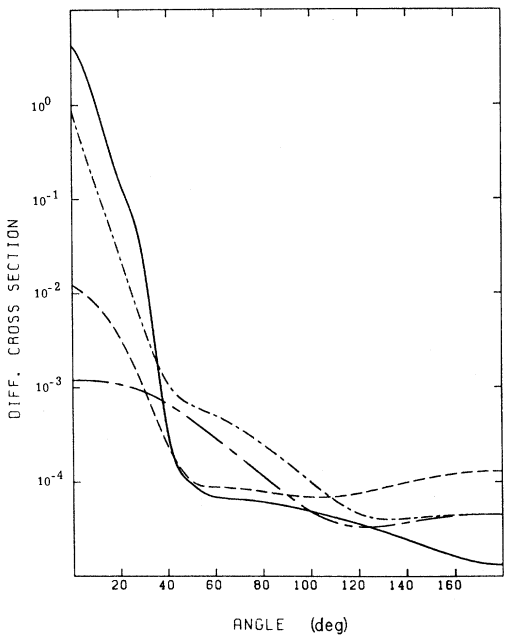

FIG. 6. Differential cross sections (in 10^{-16} cm^2/sr) for electronic excitation by 60-eV electrons. The labels are the same as in Fig. 5.

B. Dissociative processes

Electron-impact dissociation of molecules is an important basic process in atmospheric physics and laser systems. A molecule can be dissociated by electron impact when it is excited to the continuum levels of an electronic state. Such an excited state could be a purely repulsive state or a bound state with discrete vibrational levels in addition to continuum levels. Here we will discuss dissociative processes in H_2 which lead to the formation of $2s$ metastable atoms and are of the type

$$H_2 \xrightarrow{e^-} H_2^* \rightarrow H(1s)+H(2s)\ . \tag{19}$$

Only one-electron excitation processes will be considered in this study, and hence we neglect the contribution from doubly excited states[29] and predissociation.[30] The contribution of the nth excited state to the dissociative cross section is obtained in a similar fashion as in discrete transitions discussed earlier but with the summation over the Franck-Condon factors for the discrete vibrational levels replaced by an integration over the factors for the continuum vibrational levels. In this study, we neglect the contribution from the $a\,^3\Sigma_g^+$ state, since the potential-energy curve of the $a\,^3\Sigma_g^+$ state is unfavorably located for dissociative excitation.[6]

As pointed out by Chung *et al.*,[6] since the potential-energy curves of those states listed above merge at large internuclear distance with those, e.g., ($C\,^1\Pi_u$), which dissociate to the H($1s$)+H($2p$) limit, there exists the possibility of transitions between the two sets of states as the two hydrogen atoms move away from each other. However, we expect the possibility of such nonadiabatic transitions to be small in the present case. This is also shown to be the case by Mentall and Gentieu,[31] in their photodissociation experiments. Therefore, we will assume that the states listed above will lead exclusively to the production of H($1s$)+H($2s$).

The vibrational wave functions required in the evaluation of the Franck-Condon factors are obtained by numerical integration of the equation

$$\left[\frac{d^2}{dR^2}+2\mu[W-V_n(R)]\right]P_{n\nu}(R)=0\ , \tag{20}$$

where

$$P_{n\nu}(R)=\chi_{n\nu}(R)R\ , \tag{21}$$

and $\chi_{n\nu}$ is the nth vibrational eigenfunction. We use the Kolos and Wolniewicz's[32] numerical potential function for the $E(F)\,^1\Sigma_g^+$ state, and for the $B'\,^1\Sigma_u^+$ and $e\,^3\Sigma_u^+$ states we use the Rydberg-Klein-Rees (RKR) potentials.[24] Equation (20) is

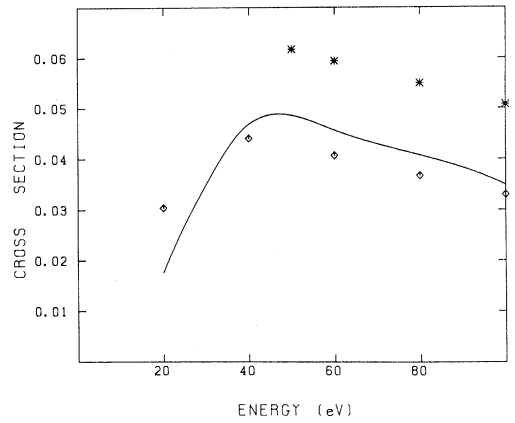

FIG. 7. Cross sections (in 10^{-16} cm^2) for electron-impact dissociation of H_2 (see text): the DW results (solid line); the Born-Ochkur-Rudge results of Ref. 6 (open diamonds) and the experimental data of Ref. 35 (stars).

solved numerically by the Numerov[33] method for the discrete vibrational wave functions, and the continuum vibrational functions are obtained following the method discussed by Morrison.[34] A grid of 0.01 a.u. is used in these integrations. The Franck-Condon factor is obtained by Simpson's rule quadrature.

In Fig. 7, we present the total dissociative cross section for the production of $2s$ atoms through the $E(F)\,^1\Sigma_g^+$, $B'\,^1\Sigma_u^+$, and $e\,^3\Sigma_u^+$ states. We also show the experimental results of Vroom and de Heer,[35] multiplied by a factor of 0.8 as suggested by Mumma and Zipf.[36] The Born-Rudge results of Chung *et al.*[6] are also shown. Our cross section agrees very well with that of the Born-Rudge approximation both in shape and in magnitude. Our calculated results account for approximately 70% of the measured cross sections. This difference is due to the other competing processes (e.g., predissociation, cascading, etc.) leading to formation of H($2s$)

TABLE II. Cross sections for production of H($1s$)+H($2s$) via the $B'\,^1\Sigma_u^+$, $E(F)\,^1\Sigma_g^+$, and $e\,^3\Sigma_u^+$ states in units of 10^{-16} cm^2.

Impact energy	$B'\,^1\Sigma_u^+$	$E\,^1\Sigma_g^+$	$e\,^3\Sigma_u^+$
20	0.014 75	0.000 64	0.002 2
30	0.032 3	0.001 4	0.001 3
40	0.044 6	0.002 2	0.000 05
60	0.044 1	0.001 57	0.000 01
100	0.034 1	0.000 82	

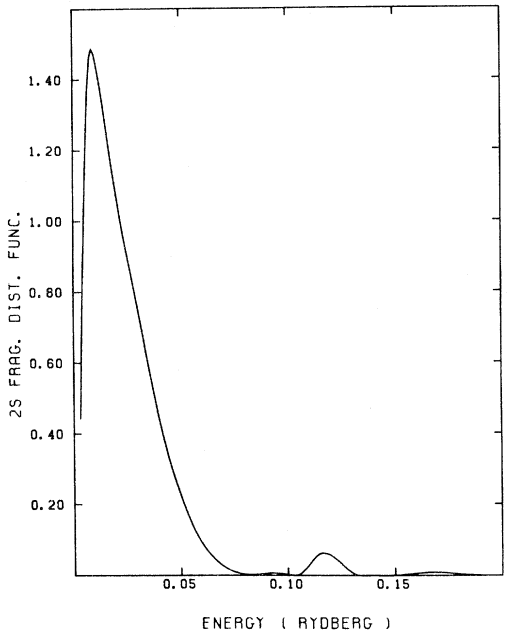

FIG. 8. Energy distribution function for H($2s$) fragments formed through electron-impact dissociation of H_2 at 40 eV.

atoms. In Table II, we present the contribution of each state to the dissociative cross section as a function of incident energy. The main contribution to this dissociative process comes for the $B'\,^1\Sigma_u^+$ state which accounts for more than 90% of the cross section in the entire energy range. The calculated cross sections for dissociation via excitation of the $B'\,^1\Sigma_u^+$ and $E(F)\,^1\Sigma_g^+$ states agree quite well with the Born-Rudge results of Chung and Lin,[6] but their cross section for dissociation through the $e\,^3\Sigma_u^+$ state is about 40 times larger than ours.

The energy distribution functions of the dissociated fragments produced by electron impact have been studied experimentally by several investigators.[37-40] Our calculated distribution function at 40 eV in the center-of-mass frame is shown in Fig. 8. One notes that the calculated distribution for the $2s$ fragments has two main features. The most important feature which contains more than 95% of the total dissociative cross section has the maximum value at about 0.005 a.u. (0.14 eV). The second feature in the calculated distribution curve has the maximum located at 0.06 a.u. (1.6 eV). The so-called fast peak observed by Spezeski *et al.*[40] with 27-eV incident electrons is peaked around 3 eV and, as expected, is not observed in this calculation.

III. CONCLUSIONS

We have calculated cross sections for various excitation and dissociation processes in H_2 by the low-energy electron impact. These cross sections were obtained within a distorted-wave approximation with the elastic scattering waves generated by the Schwinger variational method. The results are seen to be encouraging in light of their comparison with the available experimental and semiempirical results. It would be of particular interest to apply this DW method to larger molecular systems such as N_2, CO, and CO_2. Efforts in this direction are now in progress.

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